Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 1.54e-02 mol/L

Global applicability domain: Inside

Local applicability domain index: 4.77e-01

Confidence level: 5.57e-01

Nearest Neighbors from the Training Set

Image not found
Cyclopropanecarboxylic acid, 1-
(phenylsulfonyl)-, methyl ester
Measured: 5.49e-03
Predicted: 3.72e-03

Image not found
Cyclobutanecarboxylic acid, 1-
(phenylsulfonyl)-, methyl ester
Measured: 9.99e-04
Predicted: 1.53e-03

Image not found
Aldoxycarb
Measured: 4.50e-02
Predicted: 1.02e-01

Image not found
Benzenesulfonic acid, ethyl ester
Measured: 7.40e-03
Predicted: 1.03e-01

Image not found
Butoxycarboxim
Measured: 9.40e-01
Predicted: 3.25e-01